Introduction of Contaminant Analysis Program

The upgraded version of IRsolution Ver. 1.40 that will be provided with the new Fourier Transform Infrared Spectrophotometer IRAffinity-1 is equipped as standard with the “Contaminant Analysis Program (Patent Pending)”. With this program, information can be obtained with respect to not only the principle constituent of an unknown sample, but for sub-constituents that appear in the spectrum as well. Therefore, even analysts with limited experience in infrared spectroscopic analysis will find this to be a useful tool in the most difficult aspect of spectral analysis, identification and qualitative analysis. This Application News introduces the “Contaminant Analysis Program”.

■ Spectrum Search
Spectrum search (library search) is a procedure often used in contaminant analysis. This consists of using the search function included in FTIR software or specialized search software to compare the measured contaminant spectrum with spectra in a spectrum library installed on the hard drive. The comparison result is indicated with a score which represents the degree of similarity, and spectra with a high score are displayed in list (hitlist). The spectrum search is an extremely convenient function because it allows in-depth searching of similar contaminant spectra among a great number of spectra contained in the library.

However, although good results are obtained when the substance in the library is the same as contaminant, a hitlist of spectra is displayed even if the same substance is not in the library. Furthermore, the spectra contained in most commercial libraries have been obtained from analysis of pure samples of each substance, even though contaminants always occur in mixtures. Because it is only natural that a low score might be obtained when comparing a contaminant spectrum with a pure single-constituent spectrum, the contaminant principle constituent may not necessarily be ranked highest in the hit list even if it is in the library.

Therefore, it is necessary to conduct an in-depth search of spectra in the hitlist which are similar to that of the contaminant. In addition, information cannot be obtained without conducting other processing such as generating a difference spectrum, in the situation where there are second and third sub-constituents in the mixture that have a low possibility of appearing in the hit list together with the principle constituent. Thus, difficulty arises in conducting contaminant analysis when the correct answer is not obtained using a simple spectrum search.

■ Contaminant Analysis Program
The Contaminant Analysis program presents a new technique which combines spectrum search and peak matching to not only identify the principle constituent, but also indicate the possible existence of sub-constituents from very small characteristic peaks that also appear in the spectrum.

The Contaminant Analysis program includes the spectra more than 300 polymers and organic and inorganic substances obtained from analysis of common substances, and contaminant analysis is conducted based on this.
Fig. 1 and 2 show examples of analysis using this program. The analysis is conducted after the contaminant spectrum file and measurement method are specified. The analysis results are obtained. The results for the main constituent are shown in the upper field, and those for the sub-constituents are displayed in the lower field. The (+), etc. marks at the left of the constituent names indicate the analysis result, in which the greater the number of + marks (maximum 3), the higher the possibility indicated. Clicking on a substance name in the analytical result allows comparison with the contaminant spectrum. Fig. 2 shows a screen of the overlay display of the principle contaminant spectrum with the spectra of the principle constituent and sub-constituents (+++), including polyvinyl chloride (soft), calcium carbonate (CaCO3), and aluminum hydroxide (Al(OH)3). From these analytical results, it is probable that the contaminant consists of a mixture of these substances.